

# THE $3x + 1$ PROBLEM: A LOWER BOUND HYPOTHESIS

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**ABSTRACT.** Much work has been done attempting to understand the dynamic behaviour of the so-called “ $3x + 1$ ” function. In this paper, we formulate a new hypothesis that relates the minimal value of the first term in any finite sequence of iterations to the length of the sequence and the binary entropy of the “ones-ratio”. Our formulation is in agreement with all computations so far. Furthermore it implies accurate upper bounds for the total stopping time and the maximum excursion that are consistent with previous stochastic models and empirical findings.

## 1. INTRODUCTION

Let us consider the  $T$  function acting on the set of positive integers and defined by

$$(1) \quad T(n) = \begin{cases} \frac{3n+1}{2} & \text{if } n \text{ is odd,} \\ \frac{n}{2} & \text{otherwise.} \end{cases}$$

It is expected but not yet proved that, whatever the initial value of  $n$ , the repeated iterations of  $T$  reach the value 1 at some point, thus entering the infinite loop  $1, 2, 1, 2, \dots$  called the *trivial cycle*. This question is notoriously intractable, despite its simple statement, and has received various names like the  $3x + 1$  *problem*, the *Syracuse problem* or the *Collatz conjecture* [10].

**Conjecture 1.1.** ( $3x+1$  problem) *For any integer  $n > 0$ , we have  $T^{(j)}(n) = 1$  for some  $j \geq 0$ , where  $T^{(j)}$  denotes the  $j$ -th iterate of  $T$ .*

The  $3x + 1$  problem may be divided into Conjectures 1.2 and 1.3 below, asserting the absence of any other dynamic than the trivial cycle.

**Conjecture 1.2.** (Absence of divergent trajectory) *For all positive integer  $n$ , the infinite sequence  $\{T^{(k)}(n)\}_{k=0}^{\infty}$ , called the trajectory of  $n$ , is bounded.*

**Conjecture 1.3.** (Absence of non-trivial cycle) *There exist no integers  $n > 2$  and  $j > 0$  such that  $T^{(j)}(n) = n$ .*

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We propose a heuristic approach, which is greatly inspired by a well-known paper of Lagarias [8], and we mostly follow his notations and denominations throughout the paper.

Combinatorial properties of  $T$  iterations are leading us to formulate a new hypothesis (see Hypothesis 1 in §2.2) involving the binary entropy function. So far, this function rarely appears in the vast literature on the  $3x + 1$  problem with a few notable exceptions (e.g., [15, p. 84]). It has been used by Lagarias [8] to estimate the density of integers whose stopping time is bounded by a given value, thus improving a previous result of Terras [14]. Tao made a similar calculation to give a heuristic estimation of the number of non-trivial cycles, concluding that very likely there is none [13]. Let us also mention the application by Sinai of the notion of entropy of a dynamical system within a statistical modelling of the  $3x + 1$  problem [7, 12]. Besides, the binary entropy function is widely used in the context of information theory to express the entropy of Bernoulli processes.

In §3, we will see that proving our hypothesis would be more than sufficient to solve the  $3x + 1$  problem. Unexpectedly, it would further imply accurate upper bounds for the total stopping time and maximum excursion, which constitute the main result of the present paper (cf. Theorem 4.1). A brief comparison will be carried out with the predictions of the random walk model [9]. Then, in §5, we analyze a simple random model that is supporting our hypothesis.

Finally, we investigate a particular case of our hypothesis related to finite sequences of  $T$  iterations with only one even term.

## 2. A LOWER BOUND HYPOTHESIS

**2.1. Combinatorial and heuristic approach.** The  $T$  function exhibits remarkable combinatorial properties under iterations. Indeed, if we define the *parity vector* of length  $j$  of a positive integer  $n$  by setting

$$(2) \quad V_j(n) = (v_0, v_1, \dots, v_{j-1}) \quad \text{where } v_k = T^{(k)}(n) \pmod{2},$$

then we have the following result proved independently by Terras [14] and Everett [5]:

**Theorem 2.1.** (Terras) *Two positive integers  $n$  and  $m$  have same parity vector of length  $j$  if and only if  $n \equiv m \pmod{2^j}$ .*

An immediate consequence is that every positive integer  $n \leq 2^j$  is uniquely identified by its parity vector  $V_j(n)$ . Hereafter, let  $I(j, q)$  denote

the set of positive integers  $n$  for which there are exactly  $q$  occurrences of the value 1 in  $V_j(n)$ . Then, from  $I(j, q)$ , we extract the finite subset

$$(3) \quad I_0(j, q) = I(j, q) \cap \{1, \dots, 2^j\}.$$

Conversely, it follows from Theorem 2.1 that  $I(j, q)$  is the set of congruence classes modulo  $2^j$  of  $I_0(j, q)$  over the positive integers. It is easily seen that, for any fixed  $j$ , the set  $\{I_0(j, 0), \dots, I_0(j, j)\}$  is a partition of  $\{1, \dots, 2^j\}$  such that

$$(4) \quad \#I_0(j, q) = \binom{j}{q} \quad \text{for } q = 0, \dots, j$$

where  $\#$  denotes the cardinality. As an example, we exhibit for  $j = 6$  the partition of  $\{1, \dots, 64\}$ :

$$I_0(6, 0) = \{64\},$$

$$I_0(6, 1) = \{16, 20, 21, 32, 40, 42\},$$

$$I_0(6, 2) = \{4, 5, 6, 8, 10, 12, 13, 24, 26, 34, 35, 48, 49, 52, 53\},$$

$$I_0(6, 3) = \{1, 2, 3, 11, 17, 22, 23, 25, 28, 29, 36, 37, 38, 44, 45, 46, 50, 51, 56, 58\},$$

$$I_0(6, 4) = \{7, 9, 14, 15, 18, 19, 30, 33, 43, 54, 55, 57, 59, 60, 61\},$$

$$I_0(6, 5) = \{27, 31, 39, 41, 47, 62\},$$

$$I_0(6, 6) = \{63\}.$$

Lagarias suggested in [8] that the  $T$  function has some mixing properties under iteration, modulo powers of 2. One may further verify that the cumulative distribution function of  $I_0(j, q)$  from 1 to  $2^j$  appears fairly linear, for large  $j$  and  $q$  values. Therefore we may expect that the distribution of  $I_0(j, q)$  over  $[0, 2^j]$  tends to be uniform and, roughly, that

$$(5) \quad \min I_0(j, q) \approx \frac{2^j}{\binom{j}{q}}.$$

**2.2. Hypothesis.** The previous heuristic approach leads us to formulate the hypothesis to which this paper is dedicated:

**Hypothesis 1.** *There is a real constant  $C \geq 0$  such that, for all  $0 \leq q \leq j$  ( $j \neq 0$ ) and  $n \in I(j, q)$ , the lower bound*

$$(6) \quad n \geq j^{-C} \cdot 2^{(1-H(r))j}$$

*holds unless  $n = j = q = 1$ , where  $r = q/j$  is the “ones-ratio” and  $H$  is the binary entropy function defined by  $H(x) = -x \log_2(x) - (1-x) \log_2(1-x)$ .*

In the literature on the  $3x+1$  problem, the “ones-ratio” usually denotes the proportion of odd terms in a sequence leading to the value 1. Hereafter,

we extend this notion to all finite sequences of iterations, whatever the value of the last term.

The introduction of the  $H$  function in Hypothesis 1 is due to the first order approximation

$$(7) \quad \log_2 \binom{j}{q} \sim H\left(\frac{q}{j}\right) j$$

for large values of  $j$  and  $q$ , which can be derived from the Stirling formula. We recall that  $H$  is a concave function with a single maximum  $H(1/2) = 1$  and two minima  $H(0) = H(1) = 0$  by continuous extension.

The inequality (6) is sharp with  $C \approx 0$  in the two limiting cases  $q = 0$  and  $q = j$  for large  $j$  values, since  $I_0(j, 0) = \{2^j\}$  and  $I_0(j, j) = \{2^j - 1\}$ . Remarkably, it is also sharp in the central case  $j = 2q$  with  $C = 0$ . We have indeed  $\min I(2q, q) = 1$  since  $V_j(1) = (1, 0, 1, 0, \dots)$ .

In fact, Hypothesis 1 holds with  $C = 0$  in all cases where  $r = q/j \leq 1/2$ . This is a consequence of Lemma 2.2 together with the inequality

$$(8) \quad H(x) \geq 2x, \quad \text{for } x \leq \frac{1}{2}$$

which follows from the concavity of the  $H$  function.

**Lemma 2.2.** *For all  $0 \leq 2q \leq j$ ,  $\min I(j, q) = 2^{j-2q}$ .*

*Proof.* For all  $n \in I(j, q)$ , we write

$$1 \leq T^{(j)}(n) \leq 2^{2q-j} n$$

where the second inequality is easily obtained from the fact that  $T(m) \leq 2m$  for any odd integer  $m$ . It follows that

$$\min I(j, q) \geq 2^{j-2q}.$$

To complete the proof, observe that  $2^{j-2q} \in I(j, q)$ . □

As a result of Lemma 2.2 along with the strict concavity of the  $H$  function, it turns out that the crude estimate (5), which led to Hypothesis 1, is often largely erroneous when the ones-ratio is lower than  $1/2$ . Thus, inequality (6) in Hypothesis 1 is generally not sharp for long sequences of iterations with a strong downward trend. However, the numerical results in §2.3 will show that it can be quite sharp for sequences that tend to grow.

The forthcoming Theorem 2.4 states the validity of the lower bound (6) for a large set of sequences with a ones-ratio greater than  $1/2$  and lower than  $r_H = 0.609\dots$ . It relies on Lemma 2.3 below, which is a generalization of a formula by Eliahou [4] regarding all cycles of the  $T$  function.

**Lemma 2.3.** *Let  $1 \leq q \leq j$  and  $n \in I(j, q)$ . Then*

$$(9) \quad \frac{T^{(j)}(n)}{n} = 2^{-j} \prod_{k=0}^{q-1} (3 + m_k^{-1})$$

where  $m_0, \dots, m_{q-1}$  are the odd terms in the sequence  $\{T^{(k)}(n)\}_{k=0}^{j-1}$ .

*Proof.* This result is straightforward to prove by applying the same method as in [4]. Indeed, we have

$$\frac{T^{(j)}(n)}{n} = \prod_{k=0}^{j-1} \frac{T^{(k+1)}(n)}{T^{(k)}(n)} = \frac{1}{2^{j-q}} \prod_{k=0}^{q-1} \left( \frac{3 + m_k^{-1}}{2} \right)$$

since  $j - q$  is the number of even terms among  $n, T(n), \dots, T^{(j-1)}(n)$ .  $\square$

**Theorem 2.4.** *Let  $1 \leq q < j$  such that  $r = q/j \leq \rho^{-1} = 0.630\dots$ , where  $\rho = \log_2 3$ , and let  $n \in I(j, q)$  for which the terms  $n, T(n), \dots, T^{(j)}(n)$  are all distinct. Then*

$$(10) \quad n \geq j^{-\frac{1}{6}} \cdot 2^{(1-\rho r)j}.$$

Assume further that  $r \leq r_H = 0.609089767\dots$ , where  $r_H$  is the unique non-zero real number such that

$$(11) \quad H(r_H) \log 2 = r_H \log 3.$$

Then there holds the lower bound

$$(12) \quad n \geq j^{-\frac{1}{6}} \cdot 2^{(1-H(r))j}.$$

*Proof.* From Lemma 2.3, we write

$$\frac{1}{n} \leq \frac{T^{(j)}(n)}{n} = 2^{-j} \prod_{k=0}^{q-1} (3 + m_k^{-1})$$

where  $m_0, \dots, m_{q-1}$  are the odd terms among  $n, T(n), \dots, T^{(j-1)}(n)$ . This gives

$$(13) \quad \log n \geq j \log 2 - q \log 3 - \sum_{k=0}^{q-1} \log \left( 1 + \frac{1}{3m_k} \right)$$

with

$$(14) \quad \sum_{k=0}^{q-1} \log \left( 1 + \frac{1}{3m_k} \right) \leq \frac{1}{3} \sum_{k=0}^{q-1} \frac{1}{m_k}$$

by applying  $\log(1+x) \leq x$ . Since  $m_0, \dots, m_{q-1}$  are distinct odd numbers strictly greater than 1, we get

$$(15) \quad \sum_{k=0}^{q-1} \frac{1}{m_k} \leq \sum_{k=1}^q \frac{1}{2k+1}.$$

Then, from the upper bound

$$\sum_{k=1}^q \frac{1}{2k+1} \leq \frac{1}{2} \log q + \log 2 + \frac{1}{2} \gamma_{euler} - 1 + \frac{1}{2q}$$

where  $\log 2 + \frac{1}{2} \gamma_{euler} = 0.981 \dots$ , we infer

$$(16) \quad \sum_{k=1}^q \frac{1}{2k+1} \leq \frac{1}{2} \log q - \frac{1}{2} \log r = \frac{1}{2} \log j$$

for  $q \geq 3$ , using the fact that  $r \leq \rho^{-1}$ . It is easy to state inequality (16) for  $q = 1, 2$ . E.g., for  $q = 1$ , we check that

$$\frac{1}{3} < \frac{1}{2} \log 2 \leq \frac{1}{2} \log j.$$

It follows from the inequalities (13) to (16) that

$$\log n \geq j \log 2 - q \log 3 - \frac{1}{6} \log j,$$

or equivalently,

$$n \geq j^{-\frac{1}{6}} 2^{(1-\rho r)j}.$$

To conclude the proof, observe that the  $H$  function is strictly concave. This implies that there is a unique non-zero real  $r_H$  for which  $H(r_H) = \rho r_H$ , and that  $H(x) \geq \rho x$  if and only if  $x \leq r_H$ . As a result, if we further assume that  $r \leq r_H$ , it yields  $\rho r \leq H(r)$  and

$$n \geq j^{-\frac{1}{6}} 2^{(1-H(r))j}$$

as claimed.  $\square$

The condition that all terms of the sequence are distinct in Theorem 2.4 is mandatory to ensure that no cycle appears. Otherwise, the inequality (10) would be easily falsified, by considering  $n = 27 \in I(74, 43)$  for instance.

**Remark.** The value of  $r_H$  already appears in various papers of Lagarias and coauthors (e.g., [7, p. 140]) as the ones-ratio upper limit for finite sequences leading to 1 in stochastic models of the  $3x+1$  problem. Its close relationship with the  $H$  function was never mentioned so far. This topic is treated in §4.

**2.3. Numerical results.** We computed the trajectory of all integers  $n \leq 10^9$ . According to the calculations, Hypothesis 1 holds with  $C = 0$  for  $n \leq 10^9$  in all cases where  $j \neq q$ , except for a few integers  $n$  given in Table 1. The value  $c(n)$  in Table 1 denotes the smallest non-negative real such that Hypothesis 1 holds for  $n$  provided  $C \geq c(n)$ , whatever the number  $j$  of iterations. Note that for  $n = 1$ , the case  $j = 1$  is excluded.

n	j	q	q/j	c(n)
1	3	2	0.666	0.154
27	45	33	0.733	0.472
31	42	31	0.738	0.408
41	44	32	0.727	0.265
47	41	30	0.731	0.195
54	46	33	0.717	0.132
55	46	33	0.717	0.127
62	43	31	0.720	0.058
63	43	31	0.720	0.053
73	48	34	0.708	0.001
159487	35	32	0.914	0.574
212649	37	33	0.891	0.195
239231	34	31	0.911	0.293
358847	33	30	0.909	0.008
5095423	29	28	0.965	0.091
19638399	199	140	0.703	0.034
21916159	40	37	0.925	0.045
319804831	91	77	0.849	0.980
379027947	96	80	0.833	0.774
426406441	93	78	0.838	0.773
479707247	90	76	0.844	0.776
568541921	95	79	0.831	0.575
639609663	92	77	0.836	0.571
719560871	89	75	0.842	0.571
758055895	97	80	0.824	0.386
852812883	94	78	0.829	0.375
898436615	102	83	0.813	0.226
959414495	91	76	0.835	0.368

TABLE 1. Integers  $n \leq 10^9$  such that  $c(n) > 0$  and  $j, q$  values from which  $c(n)$  has been derived. All cases where  $j = q$  are omitted.

**Remark.** One may verify that  $c(n)$  exists whenever the trajectory of  $n$  contains the value 1. This follows from the fact that  $1/2$  is a critical point for the  $H$  function.

We found three successive records 0.472, 0.574 and 0.980 for the values of  $c(n)$ , corresponding to the integers  $n = 27, 159487$  and  $319804831$ , in that order. These numbers are already known as “maximum excursion” record-holders for the  $3x + 1$  problem [11] (see also §4.1). Table 2 gives the other known record-holders for the maximum excursion that are leading to non-zero values of the  $c$  function.

n	j	q	q/j	c(n)
1410123943	197	144	0.730	0.145
272025660543	109	91	0.834	0.081
871673828443	107	91	0.850	0.327
3716509988199	201	155	0.771	0.426
9016346070511	202	155	0.767	0.113
1254251874774375	227	175	0.770	0.076
10709980568908647	298	222	0.744	0.077
1980976057694848447	399	292	0.731	0.408

TABLE 2. Known maximum excursion record-holders  $n > 10^9$  for which  $c(n) > 0$ .

As a result of these calculations, if we assume Hypothesis 1, then

$$(17) \quad C > 0.98.$$

However, we previously omitted the case  $j = q$ , which occurs when  $n \equiv -1 \pmod{2^j}$ . It is obvious that  $c(2^j - 1) > 0$  for all  $j > 1$ . We found that the highest value of  $c(2^j - 1)$  for  $1 < j < 1000$  is  $c(3) = 0.415 \dots$ . Note that it may be necessary to operate more than  $j$  iterations of  $T$  to get the value of  $c(2^j - 1)$  (e.g.,  $n = 31$  or  $63$  in Table 1).

One observes, mainly in Table 1, that the integers  $n$  for which  $c(n) > 0$  tend to form “clusters” of sequences with very similar lengths and ones-ratios. This is due to a well-known phenomenon of *coalescence* of sequences. For example, the trajectories starting from 27 and 31 are almost identical since  $T^{(3)}(27) = 31$ .

### 3. BACK TO THE $3x + 1$ PROBLEM

Hypothesis 1 asserts that all integers  $n \in I(j, q)$  with  $j \neq 2q$  are lower bounded by a quasi-exponential function whose growth rate depends on the ones-ratio  $q/j$ . Moreover it implies that the ones-ratio of any given trajectory always converges to  $1/2$  as the number of iterations tends to  $\infty$ , thus maximizing the binary entropy function. Proving this property would be sufficient to solve the  $3x + 1$  problem, as shown by the next lemma.

**Lemma 3.1.** *Hypothesis 1 implies that the trajectory of any positive integer contains the value 1 ( $3x + 1$  problem).*

*Proof.* Suppose that the trajectory of a given positive integer  $n$  does not contain the value 1. We may assume, without loss of generality, that  $n$  is the smallest term in the trajectory:  $n \leq T^{(j)}(n)$  for any  $j$ .



We obtain by Lemma 2.3

$$n \leq T^{(j)}(n) \leq 2^{-j}(3 + 3^{-1})^q \cdot n$$

where  $q$  is the number of odd terms among  $n, T(n), \dots, T^{(j-1)}(n)$ . This gives

$$(3 + 3^{-1})^q \geq 2^j.$$

Therefore the ones-ratio  $r = q/j$  has lower bound

$$r \geq r_0 = \frac{\log 2}{\log(3 + 3^{-1})} = 0.575 \dots$$

and  $H(r)$  is upper bounded by  $H(r_0) = 0.983 \dots$ . It follows that the right hand side in (6) is unbounded as  $j$  tends to infinity, yielding a contradiction with Hypothesis 1.  $\square$

#### 4. DYNAMIC BEHAVIOUR

**4.1. Total stopping time and maximum excursion.** Since Crandall [3], the dynamic of  $T$  is often compared to a multiplicative random walk with a downward drift. Several stochastic models [1, 7, 9] have been proposed in order to explain the empirical observations concerning the *total stopping time*  $\sigma_\infty(n)$  and the *maximum excursion*  $t(n)$  of a trajectory starting from  $n$ . Recall that  $\sigma_\infty(n)$  is the number of iterations until the first occurrence of 1, and  $t(n)$  is the highest term of the trajectory. Hypothetically, we set  $\sigma_\infty(n) = \infty$  if the trajectory of  $n$  does not contain the value 1, and  $t(n) = \infty$  if it is unbounded. The stochastic models predict that

$$(18) \quad \limsup_{n \rightarrow \infty} \frac{\sigma_\infty(n)}{\log n} = \gamma_{RW} \approx 41.677647$$

and

$$(19) \quad \limsup_{n \rightarrow \infty} \frac{\log t(n)}{\log n} = 2,$$

which is consistent with all the empirical data provided independently by Oliveira e Silva and Roosendaal. As reported in [7], the highest known value of the ratio  $\sigma_\infty(n)/\log n$  is equal to  $36.716 \dots$ , due to the finding of a new record-holder  $n \approx 7.21 \times 10^{21}$ . The accuracy of (19) is also discussed in [7, 11], where all known integers  $n$  such that  $t(n) > n^2$  are given, starting with  $n = 27$ . At the time of writing, the verification process covers all integers  $n$  up to  $5.76 \times 10^{18}$ , thanks to various optimization techniques like the use of search trees for the preselection of congruence classes [11].

**4.2. Main result.** According to the next theorem, the expected dynamic behaviour of  $T$  under iteration, described as above, may be largely derived from Hypothesis 1, with some refinement to the second order.

**Theorem 4.1.** *Assume Hypothesis 1. Then there hold the upper bounds*

$$(20) \quad \sigma_\infty(n) \leq \gamma_H \log n + O(\log \log n)$$

and

$$(21) \quad \log t(n) \leq 2 \log n + O(\log \log n)$$

for integers  $n \geq 2$ , where

$$\gamma_H = (\log 2 - r_H \log 3)^{-1} = 41.677647655 \dots$$

and  $r_H$  defined as in Theorem 2.4.

*Proof of (20).* Let  $n \geq 2$ . Assuming Hypothesis 1, we have  $\sigma_\infty(n) < \infty$ , by Lemma 3.1. Set  $j = \sigma_\infty(n)$ , so that  $T^{(j)}(n) = 1$ .

Let  $q$  be the number of odd terms among  $n, T(n), \dots, T^{(j-1)}(n)$ .

The case  $q = 0$  is simply stated:  $n = 2^j$  and  $j = (\log 2)^{-1} \log n$ .

Consider now the case  $0 < r = q/j \leq r_H$ . Since  $n, T(n), \dots, T^{(j)}(n)$  are distinct, there holds formula (10) in Theorem 2.4, which in turn implies

$$j \leq \frac{\log n + \frac{1}{6} \log j}{(1 - \rho r) \log 2}$$

with

$$(1 - \rho r) \log 2 \geq (1 - \rho r_H) \log 2 = \gamma_H^{-1}.$$

The case  $r > r_H$  gives by assuming Hypothesis 1

$$j \leq \frac{\log n + C \log j}{(1 - H(r)) \log 2}$$

with  $C \geq 0$  a constant, and

$$(1 - H(r)) \log 2 > (1 - H(r_H)) \log 2 = \gamma_H^{-1}.$$

Thus, in all cases, we obtain the upper bound

$$j \leq \gamma_H (\log n + C \log j)$$

since  $C > 1/6$ , according to (17). It yields  $j = O(\log n)$ , and we finally get

$$\sigma_\infty(n) \leq \gamma_H \log n + O(\log \log n)$$

as claimed.  $\square$

*Proof of (21).* Let  $n \geq 3$  be an odd integer. Assuming Hypothesis 1, we have  $t(n) < \infty$ , by Lemma 3.1. Let  $j \geq 1$  such that  $T^{(j)}(n) = t(n)$ . We may suppose, without loss of generality, that  $n$  is the smallest term among  $n, T(n), \dots, T^{(j-1)}(n)$ .

Using Lemma 2.3, we get

$$\frac{t(n)}{n} \leq \frac{3^q}{2^j} \left(1 + \frac{1}{3n}\right)^q.$$

where  $q$  is the number of odd terms in the iterated sequence going from  $n$  to  $T^{(j-1)}(n)$ . Then we divide by  $n$  and apply Hypothesis 1:

$$\frac{t(n)}{n^2} \leq j^C \cdot 2^{(\rho r + H(r) - 2)j} \cdot \left(1 + \frac{1}{3n}\right)^q$$

with  $\rho = \log_2 3$  and  $r = q/j$ . Now one verifies that  $H(x) + \rho x \leq 2$  for any  $x$  where the equality holds if and only if  $x = 3/4$ . It follows that

$$\frac{t(n)}{n^2} \leq j^C \cdot \left(1 + \frac{1}{3n}\right)^q$$

and, taking the logarithm,

$$\log t(n) \leq 2 \log n + C \log j + \frac{q}{3n}$$

with the upper bound  $\log(1+x) \leq x$ . Since  $q \leq j \leq \sigma_\infty(n)$ , the inequality (20) gives the claimed result

$$\log t(n) \leq 2 \log n + O(\log \log n).$$

This completes the proof of Theorem 4.1.  $\square$

The above proof suggests that a maximum excursion record is more likely to occur when the ones-ratio of the sequence that goes from  $n$  to  $t(n)$  is approximately  $3/4$ . This prediction is in good agreement with the empirical data in Table 2, mostly for long sequences.

**4.3. From the random walk model to entropy.** Our purpose is not to discuss the existing stochastic models related to the  $3x + 1$  problem. Yet one may ask whether the constants  $\gamma_{RW}$  and  $\gamma_H$  are identical. Though they are seemingly the same, their respective definitions differ. Recall that  $\gamma_{RW}$  originated in a model described in [9], namely the *random walk model*.

For each integer  $n \geq 1$ , the authors of [9] consider a sequence of i.i.d. random variables  $X(n, k)$ ,  $k \geq 1$ , taking their values in the discrete set  $\{\log 2, \log \frac{2}{3}\}$  with the same probability  $\frac{1}{2}$ . Starting from  $\log n$ , each random variable represents a single step towards  $-\infty$  within some additive random walk on a logarithmic scale.

Using Chernoff's bound from the theory of large deviations, it was stated that almost surely

$$\limsup_{n \rightarrow \infty} \frac{\min_{k \geq 1} \left\{ k : \log n - \sum_{i=1}^k X(n, i) \leq 0 \right\}}{\log n} = \gamma_{RW}$$

where  $\gamma_{RW}$  is the unique solution with  $\gamma_{RW} > \left(\frac{1}{2} \log \frac{4}{3}\right)^{-1}$  of the equation

$$(22) \quad \gamma_{RW} \cdot g\left(\frac{1}{\gamma_{RW}}\right) = 1.$$

The rate function  $g$  above is the Legendre transform

$$(23) \quad g(a) = \sup_{\theta \in \mathbb{R}} (a\theta - \log M_{RW}(\theta))$$

defined for  $\log \frac{2}{3} < a < \log 2$ , with the moment generating function

$$M_{RW}(\theta) = \frac{1}{2} \left( 2^\theta + \left(\frac{2}{3}\right)^\theta \right).$$

We give a more simple expression of the rate function in the next lemma.

**Lemma 4.2.** *Let  $0 < r < 1$ . Then*

$$(24) \quad g(\log 2 - r \log 3) = (1 - H(r)) \log 2$$

where  $g$  is defined as in (23) and  $H$  is the binary entropy function.

*Proof.* Set  $a = \log 2 - r \log 3$  and suppose that  $\theta^*$  verify

$$g(a) = a\theta^* - \log M_{RW}(\theta^*).$$

Writing the condition

$$\frac{d}{d\theta} (a\theta - \log M_{RW}(\theta)) (\theta^*) = 0$$

leads to the relation

$$a - \log 2 + \frac{\log 3}{3^{\theta^*} + 1} = 0,$$

which simplifies to

$$r(3^{\theta^*} + 1) = 1.$$

We obtain after calculation

$$g(a) = r \log r + (1 - r) \log(1 - r) + \log 2. \quad \square$$

**Remark.** Lemma 4.2 relates the rate function to the binary entropy function. It can be derived directly by using another form of Chernoff's bound for the simple case of a Bernoulli distribution and based on the notion of relative entropy (see, e.g., [2] for this formulation).

Setting  $\gamma_{RW} = (\log 2 - r_{RW} \log 3)^{-1}$ , we get from (22) and Lemma 4.2 the expected equation

$$H(r_{RW}) \log 2 = r_{RW} \log 3$$

with  $r_{RW} > \frac{1}{2}$ . Thus,  $r_{RW} = r_H$  and  $\gamma_{RW} = \gamma_H$ , where  $r_H$  and  $\gamma_H$  are defined as in Theorems 2.4 and 4.1, respectively. The equality of both constants  $\gamma_{RW}$  and  $\gamma_H$  suggests that the implications of Hypothesis 1 are in full agreement with the predictions of the random walk model. Interestingly, the fact that  $\gamma_H$  does not depend on the value of the constant  $C$  in Hypothesis 1 further strengthens its relevance.

## 5. A RANDOM MODEL OF UNIFORM DISTRIBUTION

The heuristic assumptions made in §2.1 give no indication on the value of the constant  $C$  in Hypothesis 1. To this end, let us consider a random model<sup>1</sup> where the elements  $n \in I_0(j, q)$  are represented by a set of independent random variables  $\{X_{j,q,i} : i = 1, 2, \dots, \binom{j}{q}\}$  having a continuous uniform distribution on the interval  $[0, 2^j]$ .

Let  $P(j, q)$  denote the probability that

$$(25) \quad X_{j,q,i} < j^{-C} \cdot 2^{(1-H(r))j}$$

where  $i, j, q, r$  are taken such that  $0 \leq q \leq j$  ( $j \neq 0$ ),  $1 \leq i \leq \binom{j}{q}$  and  $r = q/j$ . The value of  $P(j, q)$  obviously does not depend on  $i$ :

$$P(j, q) = j^{-C} \cdot 2^{-H(r)j}.$$

Let us introduce the infinite sum of probabilities

$$S(C) = \sum_{j=1}^{\infty} \sum_{q=0}^j \binom{j}{q} P(j, q),$$

which estimates the number of times the inequality (25) is satisfied over all admissible values of  $i, j, q$ . By the Stirling formula, we have

$$(26) \quad \binom{j}{q} \sim \frac{2^{H(r)j}}{\sqrt{2\pi r(1-r)j}}.$$

for  $\varepsilon \leq r \leq 1 - \varepsilon$ , with  $\varepsilon > 0$  fixed. Then we get the approximations

$$\binom{j}{q} P(j, q) \sim \frac{j^{-\frac{1}{2}-C}}{\sqrt{2\pi r(1-r)j}}$$

---

<sup>1</sup>This random model is much more simple than the random walk model [9]. We point out that, in our model, the number of elements in  $I_0(j, q)$  is set to  $\binom{j}{q}$ , whereas, in the random walk model, the number of sequences of length  $j$ , starting from  $\log n$  with  $n \leq 2^j$ , and having  $q$  terms considered as “odd” is a Gaussian random variable with mean  $\binom{j}{q}$ . Yet we expect that those models lead to similar predictions regarding Hypothesis 1.

and

$$\sum_{q=0}^j \binom{j}{q} P(j, q) \sim \frac{j^{\frac{1}{2}-C}}{\sqrt{2\pi}} \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = \sqrt{\frac{\pi}{2}} \cdot j^{\frac{1}{2}-C}.$$

One may verify (e.g., by developing the Stirling series to the next order) that the latter approximation is still valid when summing on  $q$ .

We infer that  $S(C) < \infty$  if and only if  $C > 3/2$ , by considering the conditional convergence of the Riemann Zeta function on the real line. Thus, almost surely, inequality (25) occurs at most finitely many times when  $C > 3/2$ , as a consequence of the Borel-Cantelli lemma.

This simple model suggests that Hypothesis 1 is likely to be satisfied for any  $C > 3/2$  and all  $j$  sufficiently large. Nevertheless, there is no randomness in the sets  $I_0(j, q)$ , and the previous estimation of the plausible values of  $C$  may be flawed for various reasons<sup>2</sup>:

- (i) The elements of  $I_0(j, q)$  have a lower bound given by Lemma 2.2 when  $r \leq 1/2$ , and all constant  $C \geq 0$  is admissible in that case.
- (ii) The values  $\min I_0(j, q)$  and  $\min I_0(j+1, q)$  are often equal, and thus, correlated. For example,

$$\min I_0(50, 30) = \min I_0(51, 30) = 103.$$

- (iii) The values  $\min I_0(j, q)$  and  $\min I_0(j, q+1)$  are interdependent when leading to coalescent sequences after a few iterations.

Therefore, it remains plausible that Hypothesis 1 holds for a constant  $C$  lower than  $3/2$ . Yet, the exact value of  $C$  does not matter in most cases, as the first order of the lower bound (6) is the exponential term.

## 6. A PARTICULAR CASE

**6.1. Effective lower bound.** On a theoretical level, we know very little about the smallest element of the set  $I(j, q)$  in all cases where  $\log_3 2 < q/j < 1$ , which relates to sequences that tend to grow and have at least one even term. Here we briefly investigate the most simple of those cases, that is  $q = j - 1$ , for which  $\#I_0(j, j-1) = j$ .

**Lemma 6.1.** *Let  $j \geq 2$ . Then  $I_0(j, j-1) = \{n_{j,k}\}_{k=0}^{j-1}$  with*

$$n_{j,0} = 2^j - 2 \quad \text{and} \quad n_{j,k} = \left(\frac{2}{3}\right)^k (b_k(j-k) \cdot 2^{j-k} - 1) - 1$$

for  $1 \leq k \leq j-1$ , where  $b_k(l) = 2^{-l} \bmod 3^k$ . Moreover, the lower bound

$$(27) \quad \min I(j, j-1) \geq 2^{j/(1+\rho)} - 2$$

---

<sup>2</sup>See also [7, p. 153] for a similar discussion on the random walk model.

holds, with  $\rho = \log_2 3$ .

*Proof.* It is straightforward to state that the first  $j - 1$  iterates of  $n_{j,k}$  are odd integers, except  $T^{(k)}(n_{j,k})$ . We have indeed

$$T^{(k)}(n_{j,k}) = b_k(j - k) \cdot 2^{j-k} - 2$$

for  $1 \leq k \leq j - 1$ . Thus, it suffices to observe that  $1 \leq n_{j,k} \leq 2^j$  for all  $k$  to conclude that the  $j$  elements of  $I_0(j, j - 1)$  are the  $n_{j,k}$  integers.

Now we are left to prove (27). On the one hand, we can write

$$(28) \quad n_{j,k} \geq \left(\frac{2}{3}\right)^k (2^{j-k} - 1) - 1 \geq \frac{2^j}{3^k} - 2 = 2^{j-\rho k} - 2$$

for  $1 \leq k \leq j - 1$ , by using  $b_k(l) \geq 1$ . On the other,

$$(29) \quad n_{j,k} = 2^k \left( \frac{b_k(j - k) \cdot 2^{j-k} - 1}{3^k} \right) - 1 \geq 2^k - 1$$

which follows from the fact that  $(b_k(l) \cdot 2^l - 1)$  is a non-zero multiple of  $3^k$  for any  $l \geq 1$ . Putting (28) and (29) together yields

$$n_{j,k} \geq 2^{\max(k, j-\rho k)} - 2.$$

The lower bound

$$\min_{1 \leq k \leq j-1} \max(k, j - \rho k) \geq \frac{j}{1 + \rho}$$

completes the proof.  $\square$

The effective lower bound (27) is quite weak compared to Hypothesis 1 which asserts that

$$(30) \quad \min I(j, j - 1) \geq j^{-C} \cdot 2^{(1-H(1-1/j))j} \sim e^{-1} \cdot j^{-(C+1)} \cdot 2^j.$$

A simple calculation shows that the assumption (30) on the  $n_{j,k}$  integers leads to the roughly equivalent lower bound

$$(31) \quad b_k(l) \geq \frac{3^k}{e \cdot (l + k)^D} \quad \text{for all } k, l \text{ positive integers,}$$

where  $D \simeq C + 1$  is a constant. To our knowledge, proving (31) is a non-trivial problem in number theory.

As the multiplicative group  $(\mathbb{Z}/3^k\mathbb{Z})^*$  is cyclic of order  $2 \cdot 3^{k-1}$ , the  $b_k$  functions are periodic with period  $2 \cdot 3^{k-1}$ , and there holds

$$b_k(2 \cdot 3^{k-1}) = 1.$$

The inverse functions  $b_k^{-1}$  are the discrete logarithms in base  $1/2$ , modulo  $3^k$ . Thus, the hypothetical lower bound (31) may be related to the distribution of discrete logarithms [6].

**6.2. Numerical results.** In order to test numerically Hypothesis 1 in that case, we checked the lower bound (6) by setting  $q = j - 1$ ,  $n = n_{j,k}$  and  $C = 0$  for all  $0 \leq k < j \leq 10000$ . If it is falsified, which occurred 3741 times, then we computed the value of  $c(n)$ , where the  $c$  function is defined as in §2.3. Here we only give the three highest values found:

$$c(n_{85,56}) = 0.865 \dots,$$

$$c(n_{2858,1270}) = 0.817 \dots,$$

$$c(n_{5461,488}) = 0.813 \dots$$

The three above  $n_{j,k}$  integers have 22, 854 and 1637 decimal digits, in that order. Let us mention that the corresponding  $c(n_{j,k})$  values have been obtained after exactly  $j$  iterations. These numerical results do not improve the bound (17), thus supporting Hypothesis 1.

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